Mechanism of the reorientation of stripes in the cuprates

Marcin Raczkowski[a,b] Raymond Frésard[b] Andrzej M. Oleś[a,c]

[a] *Marian Smoluchowski Institute of Physics, Jagellonian University, Reymonta 4, PL-30059 Kraków, Poland*
[b] *Laboratoire CRISMAT, UMR CNRS–ENSICAEN(ISMRA) 6508, F-14050 Caen, France*
[c] *Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany*

Abstract

Using the mean field theory in the slave-boson approach we analyzed the electron correlation effects in the stripe phases. One finds that a finite next-nearest neighbor hopping t' plays an important role in the low doping regime, where it controls the crossover from the filled diagonal to half-filled vertical/horizontal stripes at doping $x \simeq 1/16$.

Key words: high temperature superconductors; Hubbard model; stripe phase; slave-boson approach

The dependence of magnetic correlations on the doping in high temperature superconductors is the subject of intense recent experimental studies [1]. They confirmed the theoretical prediction of self-organized one-dimensional structures called stripe phases [2], which act as antiphase domain walls for the antiferromagnetic (AF) order in the doped cuprates. Understanding of the stability of the half-filled vertical stripe (HVS) metallic phase versus filled diagonal stripe (FDS) insulating phase requires the analysis of electron correlation effects [3,4,5]. Here we analyze the microscopic origin of the observed reorientation from the FDS phase to the HVS one, observed in the cuprates in the low doping regime [6], within the extended Hubbard model with next neighbor (t) and next-nearest neighbor (t') hopping. The latter parameter is expected to play an important role — while the Hartree-Fock (HF) approximation predicts showed that doped holes redistribute and the kinetic energy is gained in stripe phases for increasing $-t'/t$ [7], it has been also suggested that large $-t'/t$ destabilizes the stripe order.

We implement local electron correlations within a rotationally invariant slave-boson (SB) approach in spin space [8], introducing auxiliary boson operators $\{e_i, d_i, p_{i0}, \mathbf{p}_i\}$ which control the actual electronic configuration at each site i. The Hamiltonian may be then written in the form,

$$H = -\sum_{ij}\sum_{\sigma\lambda\tau} t_{ij} z^{\dagger}_{i\sigma\lambda} f^{\dagger}_{i\lambda} f_{j\tau} z_{j\tau\sigma} + U\sum_i d^{\dagger}_i d_i, \qquad (1)$$

where $\{\underline{z}_i, \underline{z}_j\}$ are 2×2 matrices in spin space which depend on the actual configuration of the boson fields. When they are replaced by their time-independent averages using the mean-field procedure of Kotliar and Ruckenstein [9], the respective amplitudes t_{ij} for the hopping of $f^{\dagger}_{j\sigma}$ pseudofermions are renormalized.

We analyzed the stability of various possible stripe phases for the low doping $x = 1/16$. For each stripe phase we performed the symmetry analysis, defined its symmetry group, and the relevant magnetic unit cell. The self-consistent calculations for stripe phases were then completed in reciprocal space which allows one to analyze large clusters and to eliminate finite-size effects [5]. In order to reach fast convergence, the calculations were done at finite but very low temperature $\beta t = 1000$, with $\beta = 1/k_B T$, so that the free energy is approximately equal to the internal energy E.

Taking the relevant parameters for the cuprates with $U = 12t$ [3], one finds that the energy of the FDS phase is lower than that of the HVS phase (Table 1). A somewhat larger Coulomb potential energy E_U in the FDS phase is accompanied by the large gain of the kinetic energy E_t in this phase, in agreement with the

* Corresponding author; e-mail: a.m.oles@fkf.mpg.de.

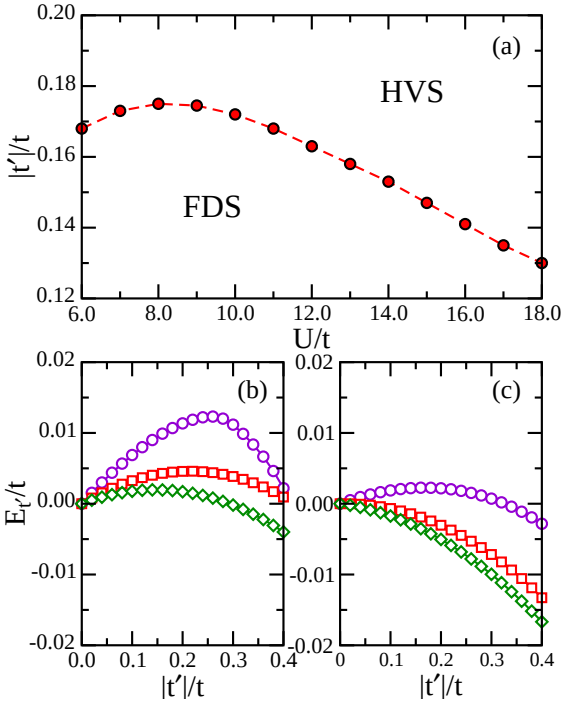

Fig. 1. (a) Phase boundary between the FDS phase and HVS phase, as obtained for increasing U/t and next-nearest-neighbor hopping $|t'|/t$. Average kinetic energy $E_{t'}$ per diagonal bond at the doping $x = 1/16$ for increasing $|t'|$ in: (b) FDS phase, and (c) HVS phase. Circles, squares and diamonds show the data obtained for $U/t = 6$, 12 and 18.

solitonic mechanism which stabilizes insulating stripe phases, so that $\Delta E = E_{\rm FDS} - E_{\rm HVS} = -0.0065t$. At finite $t' = -0.3t$, the charge redistributes and the interaction energy E_U is almost almost equal in both phases. Although the kinetic energy E_t is still lower in the FDS phase, the frustrated next-neighbor kinetic energy E'_t is paid in this phase, while it is gained in the HVS phase. As a result, the HVS phase is more stable and $\Delta E = +0.0051t$.

The crossover from FDS to HVS phase occurs at $|t'| \simeq 0.163t$ at $U = 12t$, and the critical value of $|t'|$ decreases with increasing U in the strong coupling regime of $U > 8t$, while for smaller values of U this trend is reversed (Fig. 1) in agreement with the recent HF results [7]. However, a correct treatment of strong electron correlations reduces the critical value of t' nearly twice with respect to the HF data. The transition between the FDS and HVS phase occurs mainly due to the kinetic energy term $E_{t'}$ which shows a remarkable dependence on $|t'|$, see Figs. 1 (b) and 1(c). For small $U = 6t$ the energy $E_{t'}$ first increases with increasing $|t'|$, and starts to decrease only above some finite value $t' \sim -0.2t$. Thereby, the kinetic energy $E_{t'} > 0$ for the FDS phase in a broad range of U and t', while $E_{t'} < 0$ for the HVS in the strong coupling regime of $U \geq 12t$. As a result, the total energy E of the HVS (FDS) phase decreases (increases) with increasing $|t'|$.

Table 1
Coulomb repulsion energy E_U, kinetic energies E_t and E'_t, and total energy E, all per one site, as obtained in the SB approach for the FDS and HVS phase for an 128×128 cluster. Parameters: $U = 12t$ and $x = 1/16$.

t'/t	phase	E_U/t	E_t/t	$E_{t'}/t$	E/t
0.0	FDS	0.2903	−0.7464	0.0	−0.4561
	HVS	0.2860	−0.7356	0.0	−0.4496
−0.3	FDS	0.2775	−0.7292	0.0039	−0.4478
	HVS	0.2767	−0.7225	−0.0071	−0.4529

The above dependence of the kinetic and total energies on the value of $|t'|$ is generic, and the crossover between the FDS and HVS phase is almost independent of the doping. For instance, at doping $x = 1/8$ and for $U = 12t$ one finds that the HVS phase is more stable for $|t'| > 0.171t$. This suggests that $|t'|$ increases with doping and causes a transition from the FDS to HVS phase at doping $x \simeq 1/16$. Hence our findings pose an interesting physical problem for future studies — microscopic derivation of the parameters of the extended Hubbard model relevant for the cuprates.

In summary, we have identified the microscopic origin of the reorientation of the domain walls, observed in the cuprates at increasing doping. By evaluating individual kinetic energy and Coulomb energy terms, we established that t' plays an important role in the low doping regime, where it controls the crossover from FDS to HVS phase. Therefore, in spite of the robust stability of FDS phase at $t' = 0$, the HVS phase takes over for the realistic value of $t' = -0.3t$ in the cuprates.

This work was supported by the Polish Ministry of Science and Education under Project No. 1 P03B 068 26, and by the Ministère Français des Affaires Etrangères under POLONIUM 09294VH.

References

[1] M.A. Kastner et al., Rev. Mod. Phys. **70** (1998) 897.

[2] J. Zaanen, O. Gunnarsson, Phys. Rev. B **40** (1989) 7391.

[3] M. Fleck, A.I. Lichtenstein, A.M. Oleś, Phys. Rev. B **64** (2001) 134528.

[4] G. Seibold, J. Lorenzana, Phys. Rev. B **69** (2004) 134513.

[5] M. Raczkowski, R. Frésard, A.M. Oleś, Phys. Rev. B **73** (2006) 174525.

[6] M. Fujita *et al.*, Phys. Rev. B **65**, (2002) 064505.

[7] M. Raczkowski, A.M. Oleś, R. Frésard, Phys. Status Solidi B **243** (2006) 128.

[8] R. Frésard, P. Wölfle, Int. J. Mod. Phys. B **6** (1992) 685.

[9] G. Kotliar, A.E. Ruckenstein, Phys. Rev. Lett. **57** (1986) 1362.